

B-5

USSR/ Physical Chemistry - Crystals

Abs Jour : Referat Zhur - Khimiya, No 4, 1957, 10929

analogous to polyhedrons in structures of PtSn_4 , PdPb_4 , AuSn_4 , CuAl_2 , CoGe_2 . Bi atoms have coordination number 11 (9 atoms Bi and 2 atoms Rh). Interatomic distance Bi-Rh is 2.80 Å, and is less by 3% than sum of atomic radii. Distance Bi-Bi is from 2.80 to 3.50 Å; three of them are close to least distance, and six to greatest distance in pure Bi. The question concerning analogy in structure of alpha-Bi₄Rh and garnet $\text{Ca}_2\text{Al}_2\text{Si}_3\text{O}_12$ is discussed.

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ZHDANOV, G. S.

AUTHOR
TITLE
PERIODICAL

KINCHIN, G.H., PEASE, R.S.

PA - 2040

The Displacement of Atoms in Solids under the Effect of Radiation. (Russian)
Uspekhi Fizicheskikh Nauk, 1956, Vol 60, Nr 4, pp 590-615 (U.S.S.R.)

Received 1/1957

Reviewed 3/1957

ABSTRACT

This is the Russian translation of articles 2 and 3 of the survey by the above mentioned authors (under the editorship of G.S.ZHDANOV), Reports on Progress in Physics, 18, 1 (1955), this survey is arranged as follows.

I. The production of displaced atoms. 1) energetical deliberations. The energy of displacement. (It is to be expected that an energy that is higher than 5 eV is needed for the displacement of an atom from its position in the lattice of a solid, the threshold values of radiation energy are given in a table for the displacement energy of 25 eV which is assumed for all further cases). 2) The number of displaced atoms. The moved atoms, bases of the theory, collisions of solid spheres, Rutherford's collisions, moved atoms which are slowed down to a full stop, fast neutrons, electrons, gamma rays. 3) The distribution of the displaced atoms and vacancies.

a) The models based upon the investigation of collisions. b) "displacement wedges" and "thermal wedges". 4) Effects in compounds. Collisions that lead to the displacement of atoms, dissolution of order.

II. Restoration of defects. In most cases the physical properties return to their original values if the temperature of the sample is increased after irradiation. As a rule it may be expected that also in the case of irradiation a certain restoration of defects takes place by heating, usually in several stages with different values of activation energy in

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PA - 2040
The Displacement of Atoms in Solids under the Effect of Radiation.

the various temperature intervals. The course taken by the restoration process may be described by the equation $dn/dt = -cn\gamma \exp(-\epsilon/kT)$. Here "n" denotes the number of the defects participating in the restoration process, ϵ the activation energy, γ the so-called "order of reaction". The II. section is arranged as follows. 1) Recombination of impressed atoms and vacancies. Pairs of atoms and vacancies located close to each other, the disordered distribution of impressed atoms and vacancies. 2) Additional processes 3) the accumulation of destructions 4) saturation 5) Annealing by radiation.

ASSOCIATION
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Not given
Library of Congress

ZHDANOV, G. S. and VLASENKO, V. I.

The National Committee for Crystallography of the USSR, Moscow-

"Automatic Synthesis of Two-Dimensional Crystal Structure Patterns"
(Section 1(1)-8, a paper submitted at the General Assembly and International
Congress of Crystallography, 10-19 Jul 57, Montreal, Canada.

C-3,800,89

ZHDANOV, G. S. (Prof.)

"The Work of the Electronic Computing Machine "Kristall" and demonstrated it."

report presented at Scientific Conference at the Inst. for Physical Chemistry
imeni L. Ya. Karpov, Acad. Sci. USSR, Nov 1957.

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24/11/NOV 68.

VLASENKO, V. I.; ZHDANOV, G. S.; SOKOLOV, A. D.

Dynamic method for analog representation of two-dimensional
functions. Priborostroenie no. 6:11-14 1957. (MIRA 10:7)
(Electronic calculating machines) (Mathematical models)

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CIA-RDP86-00513R002064620006-5"

ZHDANOV, G.S.

AUTHOR: Ozerov, R.P., Gol'der, G.A. and Zhdanov, G.S. 70-2-3/24

TITLE: An X-ray structural investigation of the oxygen vanadium bronzes of sodium and potassium $Me_0.33V_2O_5$. (Rontgenograficheskoye issledovaniye struktury kislorodnykh vanadiyevykh bronz natriya i kaliya $Me_0.33V_2O_5$.)

PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol. 2, No. 2, pp. 217-225 (U.S.S.R.)

ABSTRACT: Experimental. The valency state of V in bronzes and in vanadium-sulphur-oxygen catalysts is particularly of interest. Crystals of composition $(K,Na)_2O_2V_2O_4 \cdot 5V_2O_5$ were obtained as black laths having a blue metallic lustre. They showed a large number of faces including the simple forms 102, 101, 100, 001 variously developed. X-ray photographs assigned them to the Laue class $2/m = C_{2h}^1$. Weissenberg and oscillation photographs (11.456 cm diameter camera) with Fe radiation gave unit cell dimensions $a = 10.039$, $b = 3.605$, $c = 15.335 \text{ \AA}$ (all $\pm 0.003 \text{ \AA}$) and $\beta = 109^{\circ}12' \pm 3'$, for the sodium compound $Na_0.33V_2O_5$. This gives $V = 524.2 \text{ \AA}^3$. The compound $K_2V_2O_5$ had $d_{\text{obs.}} = 3.57 \text{ g/cm}^3$ making $z = 1 (0.97)$. $d_{\text{calc.}}$ is then 3.60.

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70-2-3/24
An X-ray structural investigation of the oxygen vanadium
bronzes of sodium and potassium $Me^{0.33}V_2O_5$. (Cont.)

The possible space groups (from the extinctions) were $A2/m$, $A/2$ and Am . On the basis of a knowledge of the crystal chemistry of the oxides of V, Mo and W and of the W bronzes the group $A2/m$ was chosen. This is confirmed by the dimension b which leads to the expectation of octahedra or trigonal bipyramids (see R.P. Ozerov - Usp. Khim. 24, 951, 1955). Using Mo radiation 800 reflections were measured from retigraph pictures using comparison scales. No extinction corrections were applied. $P(x, z)$ was constructed. A.D. Wadsley's determination of the structure of $Na_{2-x}V_6O_{15}$ helped in solving this Patterson projection. Projections for both Na and K bronzes were constructed. Several atoms overlap and this was one reason for repeating Wadsley's work. The Fourier section at $y = 0$ was calculated giving co-ordinates for the K bronze very close to those found by Wadsley (Acta Crystallography, 8, 695, 1955) for the Na bronze. A table of interatomic distances is given. Slight differences naturally occur in the $Me-O$ distances (as observed for K bronze first followed by Wadsley's value for the Na bronze); $Me-O_8$ (2.50, 2.46); $Me-O_8$ (2.49, 2.75); $Me-O_4$ (2.56, 2.51);

Card 2/3

70-2-3/24

An X-ray structural investigation of the oxygen vanadium bronzes of sodium and potassium $\text{Me}_{0.33} \text{V}_{2.5} \text{O}_5$. (Cont.)

Me-O_6 (2.57, 2.51); Me-Me (1.68, 2.22). The geometry of the structure is discussed. The structure is built from strongly distorted VO_6 octahedra. The distortion is so great that certain groupings are better regarded as trigonal bipyramids. The polyhedra differ greatly among themselves V-O distances oscillating to 1.55, 1.79, 1.89, 2.00 and 2.68 Å. There is a strong correspondence with the structure of the V oxides. The alkali atoms lie in canals between the octahedra each surrounded by seven oxygens. Seven-fold co-ordination is rare but is also found in the ion $(\text{NaF}_7)^{-2}$ and in Bi_2Ni .

Card 3/3 There are 5 figures, 2 tables and 20 references, 10 of which are Slavic.

ASSOCIATION: Ya.V. Samoylov Scientific Institute for Fertilisers and Insecto-fungicides. (Nauchnyy Institut po Udobreniyam i Insektofungisidam im Ya.V. Samoylova)

SUBMITTED: September 21, 1956.

AVAILABLE: Library of Congress

ZHODANOV, G. S.

AUTHOR: Zhdanov, G.S., Zhuravlev, N.N., Stepanova, A.A. and
Umanskiy, M.M. 70-2-16/24TITLE: The crystal chemistry of metal hexaborides. (Kristallo-
khimiya gekseboridov metallov)PERIODICAL: "Kristallografiya" (Crystallography), 1957, Vol.2,
No.2, pp. 289-290 (U.S.S.R.)

ABSTRACT: The MeB_6 structure consists of a three-dimensional framework of B atoms with Me atoms in the interstices and is formally like the CsCl structure with B₆ and Me units. In group II, Be, Mg, Ca, Sr and Ba form hexaborides as do Y, La, Ce, Pr, Nd, Gd, Er, Yb in group III. The formation by the remaining lanthanides and by Sc of hexaborides can also be predicted. In group IV, SiB₆ and ThB₆ are known. When the unit cell sizes are plotted against atomic radii the compounds fall into three series corresponding to the three groups. Coefficients of thermal expansion of CaB₆ and SiB₆ have been measured by X-ray diffraction (5.9 and 6.5×10^{-6} , respectively and are added to the measurements already made (A.A. Stepanova and M.M. Umanskiy, Trudy soveshchaniya po khimii bora i ego soedineniy. Fiz.-Khim. in-t. im. Karpova, 1955) for Ce, La and Ba (7.3, 6.4 and 6.8×10^{-6} , respectively). The coefficient

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AUTHOR: Zhdanov, G.S. 70-3-6/20
Vlasenko, V.I. and Zhdanov, G.S.

TITLE: Automatic synthesis of two-dimensional crystal structure
patterns (Avtomlicheskiy sintez dvumernykh izobrazheniy
atomnykh struktur)

PERIODICAL: "Kristallografiya" (Crystallography), 1957,
Vol. 2, No. 3, pp. 358 - 365 (U.S.S.R.)

ABSTRACT: By means of high speed digital computers it is possible
to summate Fourier series and thus compute numerical tables
within a short time. However, digital computers are unsuitable
for further analysis. The first problem is to convert the numerical
tables into a more readily usable form.

The simplest method of this synthesis is the construction
of a mosaic image. In this case each number in the table is
replaced by a round or a square spot with the colour corres-
ponding to this number. The whole of the colour spots gives
a visual mosaic image of the electron density. This is due
to the ability of the eye to integrate discrete elements in
smooth forms.

Another method is that of the model section; it is a
better method but a more difficult one. In this case it is
necessary to construct a model of the two-dimensional function

Card 1/3

Automatic synthesis of two-dimensional crystal structure patterns. (Cont.)

70-3-6/20

of the electron density, then to dissect the model with a series of planes parallel to XY on different levels and to register on a flat screen the intersection lines.

The model is constructed by two-dimensional interpolation first along the X axis, and then along the Y axis. The results of the first (X-axis) interpolation is recorded in a special storage device and represents the initial data for the second (Y axis) interpolation.

The first interpolation is performed by electronic circuits, the results being recorded in parallel circular tracks on a rotating magnetic drum. The second (Y axis) interpolation of these results, along the drum axis, as well as all other operations are also made by the electronic circuits.

The results of the second interpolation can be considered as being a curve, representing the distribution of electronic density along the Y axis (drum axis). An amplitude discriminator automatically dissects this curve parallel to the Y axis by a series of straight lines, representing the given set of electron-density values. The intersection points are recorded as light spots on a CRT screen whereby the coordinates of these spots correspond to the position of the

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70-3-6/20

Automatic synthesis of two-dimensional crystal structure patterns. (Cont.)

intersection points. Thus, during one revolution of the magnetic drum the light spots form dotted lines, representing the whole electron-density map.

The use of the magnetic drum and electronic circuits for the above mentioned purposes allows obtaining an electron-density map on a CRT screen within a few seconds after ending the summation of the Fourier series on the high-speed computer.

There are 8 figures and 7 references, 2 of which are Slavic.

ASSOCIATION: Physico-chemical Institute im. L.Ya.Karpov.
(Fiziko-khimicheskiy Institut im. L.Ya. Karpova)

SUBMITTED: February 22, 1957.

AVAILABLE: Library of Congress
Card 3/3

AUTHORS: Zhdanov, G.S., Solov'yev, S.P. and Venevtsev, Yu.N. 70-5-12/31
 TITLE: The Structural Coefficients of the Internal Field in Ferro-
 electrics with the Perovskite-type Structure. (Strukturnyye
 koeffitsiyenty vnutrennego polya v segnetoelektrikakh so
 strukturoy tipa perovskita)

PERIODICAL: Kristallografiya, 1957, Vol.2, No.5, pp. 639-645 (USSR)

ABSTRACT: Data published in the literature for the values of the structural coefficients of the internal field in perovskite-type crystals are critically examined. Relations are set up between the idealised cubic perovskite and the cases in which there are dipoles in the [001], [011] or [111] directions. The structural coefficients are calculated for the tetragonal cell of PbTiO_3 at room temperature taking account of the ionic displacements.

The field at the i-th ion is:

$$E_i = E + \sum_{k=1}^m \left(\frac{4\pi}{3} + c_{ik} \right) p_k$$

where m is the number of sub-lattices each consisting of the ions of the k-th sort, E is the external field, p_k is the

Card 1/4

70-5-12/31

The Structural Coefficients of the Internal Field in Ferroelectrics
with the Perovskite-type Structure.

dipole moment of the k-type of ions, C_{ik} are the structural coefficients. In the case where the dipoles are in the z-direction:

$$C_{ik} = \sum_j \frac{2z_{jk}^2 - x_{jk}^2 - y_{jk}^2}{(x_{jk}^2 + y_{jk}^2 + z_{jk}^2)^{5/2}}$$

where x_{jk} , y_{jk} , z_{jk} are the co-ordinates of the j-th dipole of the k-th sort relative to a dipole of the i-th sort and summation is over each dipole of the k-th sort. For the cubic cell, the C_{ik} can be expressed in terms of two quantities P and Q. The values which various authors find for these values are compared, the best values being $P = -15.04102/V$ and $Q = 4.33387/V$ as found by McKeehan (Phys. Rev. 43, 913, 1933 and 72, 78, 1947).

Card2/4

70-5-12/31

The Structural Coefficients of the Internal Field in Ferroelectrics
with the Perovskite-type Structure.

$$C_{ik} = \begin{matrix} 0 & 0 & -2Q & Q & Q \\ 0 & 0 & -2P & P & P \\ -2Q & -2P & 0 & Q & Q \\ Q & P & Q & 0 & -2Q \\ Q & P & Q & -2Q & 0 \end{matrix}$$

There are 5 sub-lattices for the ABO_3 formula. C_{ik} are the values for the truly cubic cell.

Where the distortions of the cubic cell are small (1%) the C_{ik} are different from the C_{ik} only by 2-3%. Even for $PbTiO_3$, where the distortions are large, these do not differ by more than 20%. The actual values of the coefficients for tetragonal $PbTiO_3$ where $c/a = 1.064$ are calculated and tabulated with those of McKeehan (cubic, by Ewald's method) and of Hagendorf ($BaTiO_3$ with $c/a = 1.010$) (Zeit.f.Physik, 133, 394-421, 1952). There are 1 figure, 3 tables and 14 references, 2 of which are Slavic.

ASSOCIATION: Karpov Physico-chemical Institute
(Fiziko-khimicheskiy Institut im. L.Ya. Karpova)

Card 3/4

70-5-12/31

The Structural Coefficients of the Internal Field in Ferroelectrics
with the Perovskite-type Structure.

SUBMITTED: May 31, 1957.

AVAILABLE: Library of Congress

Card 4/4

ZHDANOV, G.S.

EPEL'BAUM, V.A.; SEVAST'YANOV, N.G.; GUREVICH, M.A.; ORMONT, B.Y.; ZHDANOV,
G.S.

Phases formed in the system chromium -- boron. Part 1: Formation
of "β-chromium" under the influence of small additions of boron.
Zhur. neorg. khim. 2 no.8:1848-1854 Ag '57.
(Chromium) (Boron) (MIRA 11:3)

ZHDANOV, G.S., professor.

Scientific works by the Department of Solid State Physics. Vest.Mosk.
(MLRA 10:8)

un. 12 no.1:195-196 '57.
(Solids)

ZHDANOV, G.S.

Atomic structure and chemical bonding. Vest. Mosk.un.Ser.mat.
mekh.astron. fiz. khim. 12 no.4:61-78 '57. (MIRA 11:5)

1.Kafedra fiziki tverdogo tela Moskovskogo gosudarstvennogo
universiteta. (Chemical bonds) (Atoms)

ZHDANOV, G.S.

AUTHORS:

Venevtsev, Yu.N. and Zhdanov, G.S.

TITLE:

Crystallochemistry of Ferroelectrics of Perovskite Structure. (Kristallokhimiya sagnatoelektrikov so strukturey tipa perovskita)

PERIODICAL:

Izvestiya Akademii Nauk SSSR, Vol. XXI, #2, pp 275-285, 1957, USSR, Seriya fizicheskaya

ABSTRACT:

The data available on some ferroelectrics and anti-ferroelectrics make it presently possible to classify these compounds by their structural properties and to determine relations between the structure and the character of spontaneous elec polarization.

For crystallic structure of ferroelectrics with ABO_3 composition of the perovskite type, the existence of BO_6 octahedrals joined by their vertices is a characteristic feature; empty gaps between them are occupied by A-type ions.

The structure of the perovskite type depends mainly up on the ratios of radii of constituent ions. The valence of A ions may be 1,2,3 and that of B ions

Card 1/5

TITLE:

Crystalllochemistry of Ferroelectrics of Perovskite Structure. (Kristallokhimiya segnetoelektrikov so strukturoy tipa perovskita)

- 5,4,3 respectively. When A ions and oxygen ions have equal radii, these ions form a densely packed cubic structure. Within the oxygen octahedrals of this structure, B-ions may possess a maximum radius equal to 0.414 of the oxygen ion radius, i.e. 0.56 A. Thus an ideal contact of adjacent ions takes place when the ratio $t = \frac{r_A + r_B}{\sqrt{2}(r_A + r_B)}$ is equal to 1.

According to Megaw (8) and Naray-Szabo (9) it is sufficient to take into account co-ordination numbers of ions for evaluating the factor t by the formula:

$$t = \frac{R_A(12) + R_B}{\sqrt{2}(R_A + R_B)}$$

where R_A , R_B and R_O are tabular values of A, B, O ion radii, and subscript (12) means tabular value of the A ion radius corrected for the case of co-ordination number 12.

Card 2/5

TITLE:

Crystalliochemistry of Ferroelectrics of Perovskite Structure. (Kristallokhimiya segnetoelektrikov so strukturoy tipa perovskita)

Peculiar properties of BaTiO_3 are connected with the fact that the titanium ion has a "free" space in the BaTiO_3 cell. The main condition for the ferroactivity of an ion is that free space in the cell must be available.

Classification results of ferroelectrics and antiferroelectrics of the BaTiO_3 group are presented in Table 1. Inspection of this table shows a definite regularity between the t -value and elec polarization character. If t has a value considerably less than 1, the compound has antiferroelectric properties.

Ferroactive cations (A or B) are displaced at a certain temperature (lower than Curie point) from their symmetric positions and thereby bring about the polar rebuilding of the whole cell.

Card 3/5

TITLE:

Crystallochemistry of Ferroelectrics of Perovskite Structure. (Kristallokhimiya segnetoslektrikov so strukturoy tipa perovskita)

Displacements of B and A ferroactive cations are observed along the axes of the 2nd and 3rd and 4th orders, which result in monoclinic, rhombohedral and tetragonal distortions respectively. In the cells of antiferroelectrics, antiparallel displacements of ferroactive A cations along the axis of the 2nd order are observed.

Co-ordination numbers of A and B ferroactive cations characterizing their displacements along various axes are given in Table 2.

Ferroelectrics with $t > 1$ and accompanied by temperature changes perform 3-phase transitions. Ferroelectric $PbTiO_3$ with $t < 1$ and lowering of the temperature performs only a one-phase transition. None of the known ferroelectrics and antiferroelectrics with $t < 1$ has shown, thus far subsequent displacements of the A

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TITLE: Crystallochemistry of Ferroelectrics of Perovskite Structure. (Kristallokhimiya segnetoelektrikov so strukturoy tipa perovskita)
cation along the 3 possible directions of displacements.
Ferroelectrics possessing the perovskite structure are compounds with principally ionic character of bonds.
The article given 3 figures and 2 tables. The bibliography contains 46 references, of which 10 are Slavic and 1 Hungarian.

INSTITUTION: Physico-Chemical Institute imeni L.Ya. Karpov

PRESENTED BY:

SUBMITTED: No date

AVAILABLE: At the Library of Congress.

Card 5/5

ZHIDANOV, G.S.

5(2)

PHASE I BOOK EXPLOITATION

SOV/1916

Vsesoyuznoye soveshchaniye po khimii bora, 1955

Bor; trudy Konferentsii po khimii bora i yego soyedineniy (Boron; Transactions of the Conference on the Chemistry of Boron and Its Compounds) Moscow, Goskhimizdat, 1958. 189 p. Errata slip inserted. 2,400 copies printed.

Ed.: G.P. Luchinskiy; Tech. Ed.: M.S. Lur'ye.

PURPOSE: This book is intended for chemists, as well as for industrial personnel working with boron and its compounds.

COVERAGE: This collection contains 24 studies on the chemistry, crystalline structure, physicochemical properties, and technology of boron and its compounds. Twenty-two of the studies were presented at the All-Union Conference on Boron Chemistry, held at the Nauchno-issledovatel'skiy fiziko-khimicheskiy institut im. L. Ya. Karpova (Scientific Research Physicochemical Institute im. L. Ya. Karpov) in

Card 1/6

Boron; Transactions of the Conference (Cont.) Sov/1916

December 1955. Two of these articles deal with the thermo-chemistry of boron. The two studies on "borundum" production are being published for the first time. The studies are well illustrated and accompanied by bibliographies.

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Polyak, A.M., Ye. N. Pinayevskaya, G.B. Romov,
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AVAILABLE: Library of Congress

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6-22-59

Card 6/6

AUTHOR:

Preobrazhenskiy, Yu.A., Zhdanov, S.S.

113-58-7-2/25

TITLE:

The Economy of Smelt-Model Casting (Ob ekonomike lit'ya po vyplavlyayemym modelyam)

PERIODICAL:

Avtomobil'naya promyshlennost', 1958, Nr 7, pp 4-5 (USSR)

ABSTRACT:

In 1956, NIITAvtoprom established a catalogue of 500 individual parts used in automobile, motorcycle and bicycle production. Reduction of this list to 175 parts is possible by a very accurate method of evaluation. First, the parts are grouped by weight, intricacy and design, and the possibility of reducing the amount of mechanical machining is considered. Accurate casting to desired shape must then be effected wherever it is possible. The economy obtained by smelt-model casting of rocker arm yokes is demonstrated in a table. In the automobile building industry, this economy, by the smelt-model casting process, applies to forgings and rolled iron parts of up to 350 grams, which are later subjected to machining by cutting. In most cases, a transfer of parts made of machined rods to automats or semi-automats does not pay. The introduction of shell casting in the Moskovskiy zavod malolitrazhnykh avtomobiley (Moscow Light Car Plant) has resulted in a reduction of operators and a diminished consumption of electric

Card 1/2

The Economy of Smelt-Model Casting

113-58-7-2/25

power. There is 1 table.

ASSOCIATION: NIITAvtoprom (NIITAvtoprom)

1. Metals—Casting 2. Castings—Economic aspects

Card 2/2

70-3-2-1/26

AUTHORS: Vlasenko, V.I. and Zhdanov, G.S.

TITLE: Optical Methods of Summing Fourier Series (Opticheskiye metody summirovaniya ryadov Fur'ye)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 135 - 140 (USSR)

ABSTRACT: The various optical methods of summing Fourier series are classified according to their characteristics: sequential simultaneous, one mask/ set of masks, white/ coloured light, cinematographic/static. The properties of the photographic materials used in the Bragg-Huggins masks and in the von Eller photosommateur are discussed with reference to range of linearity and to maximum density. A new method (possibly not yet realised) is described. The Huggins masks, translated to give correct phases, pass in turn before a lamp (presumably modulated) in rapid succession so that all merge, owing to the persistence of vision, to give a summation. Cinema technique is required for this apparatus but it uses only one projecting lens and the resulting summation can be very easily recorded photographically. A machine where each mask is projected simultaneously onto a white screen and the resulting pattern of weak or strong illumination/represents the summation is also described, but appears rather impracticable. The von Eller machine is commended.

Optical Methods of Summing Fourier Series

70-3-2-1/26

There are 4 figures and 12 references, 5 of which are Soviet,
4 French and 3 English.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(Physico-chemical Institute, im. L.Ya. Karpov)

SUBMITTED: February 1, 1957
Card 2/2

AUTHORS: Verbitskaya, T.N., Zhdanov, G.S., Venevtsev, Yu.N. 70-3-2-9/26
and Solov'yev, S.P.

TITLE: Electrical and X-ray Investigations of the System
 BaTiO_3 - BaZrO_3 (Elektricheskiye i rentgenograficheskiye
issledovaniya sistemy BaTiO_3 - BaZrO_3)

PERIODICAL: Kristallografiya, 1958, Vol. 3, Nr 2, pp 186 - 196
(USSR).

ABSTRACT: Various solid solutions of BaTiO_3 - BaZrO_3 were prepared, having up to 30 mol% of the latter, by heating appropriate mixtures of BaCO_3 , TiO_2 and ZrO_2 at $1400 \pm 10^\circ\text{C}$. The resulting materials were examined by the Debye-Scherrer method with a camera of diameter 11.4 cm and Cr or Cu radiation. With Cr radiation the lines 310 and 222 occur at a sufficiently high angle to give accurate cell dimensions. (For Cu radiation the appropriate lines are 501 and 431). The significance of the splitting of the lines under the distortions observed is explained. Dimensional measurements were made to $\pm 0.001 \text{ \AA}$, monoclinic angle to $\pm 1.5'$, rhombohedral angle to $\pm 1'$ and axial ratio to ± 0.0005 . Card 1/3 For the pure compounds the cell dimensions were found to be:-

70-3-2-9/26
Electrical and X-ray Investigations of the System BaTiO_3 - BaZrO_3

BaTiO_3 , $a = 3.990$, $c = 4.027$, $c/a = 1.0093$, $V = 64.12$; and BaZrO_3 , $a = 4.386$ and $V = 73.35$. From 0 to 2 mol% of zirconate the dimensions of the tetragonal phase approached each other slightly. From 2 to 6.5% the solid solution was pseudo-monoclinic with $a = c$ and the monoclinic angle decreasing from $90^\circ 08.5'$ to $90^\circ 04.0'$. From 6.5 to 20 mol%, the solution was rhombohedral with the rhombohedral angle equal to $89^\circ 57'$ and increasing from 4.0177 to 4.0440 . Above 20% the solution was cubic with an increasing from 4.0447 to 4.0616 at 30%. Over the whole range the volume of the unit cell increased linearly from 64.12 to 67.00 \AA^3 with no breaks at the phase transitions. In pure BaTiO_3 three phase transitions (all with hysteresis) are observed on changing its temperature. They are at 120° , $0-5^\circ$ and -70 to -80°C . These transition points were measured for a range of compositions. Below 10% zirconate all four phases occur at appropriate temperatures, between 10 and 15% there is a confused region and above 15% only the cubic and rhombohedral phases occur. Measurements were also made of the dielectric constant of the material at various temperatures

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70-3-2-9/26
Electrical and X-ray Investigations of the System BaTiO_3 - BaZrO_3

and compositions.

The phase diagram constructed is like that found for BaTiO_3 - BaSnO_3 by Smolenskiy and Isupov (DAN, 1954, Vol 96, 53) and not like that drawn up by Kell and Hellicar (Akustika, 1956, Vol 6, Nr 2, p 232).

There are 8 figures, 2 tables and 26 references, 10 of which are Soviet, 2 German and 14 English.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(Karpov Physico-chemical Institute) and NII MRTF

SUBMITTED: July 18, 1957

Card 3/3

AUTHORS: Yezhkova, Z.I., Zhdanov, G.S., and Umanskiy, M.M. 70-3-2-18/26

TITLE: X-ray Determination of the Thermal Expansion Coefficients of
Guanidine Aluminium Sulphate Hexahydrate - $C(NH_2)_3[Al(H_2O)_6] \cdot [SO_4]_2$ - (GASH) (Rentgenograficheskoye opredeleniye
koeffitsiyentov termicheskogo rasshireniya guanidin-alyuminiy-
sul'fata geksagidrata - $C(NH_2)_3[Al(H_2O)_6] \cdot [SO_4]_2$)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 231-232 (USSR)

ABSTRACT: The lattice parameters of GASH at $25^{\circ}C$ were found to
be $a=11.7159 \pm 0.0007$ KX, $c=8.9335 \pm 0.0007$ KX and the
coefficients of thermal expansion were determined as
for the a axis, $\alpha_{perp.} = 10.0 \pm 0.4 \times 10^{-6}$ per deg. C

for the c axis, $\alpha_{par.} = 93.3 \pm 1.0 \times 10^{-6}$ per deg. C

The expansion was measured over the range $25-55^{\circ}C$. The 13.0.0.
Card/1 reflections were used with Cu and Fe radiations,
respectively. There are 1 figure and 2 Soviet and 2 English refs.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet im. M.V. Lomonosova
(Moscow State University im. M.V. Lomonosov)
SUBMITTED: July 3, 1957.

AUTHORS: Belov, N.V., Belyayev, L.M., Bokiy, G.B., Bronnikova, Ye.G.,
Vaynshteyn, B.K., Zhdanov, G.S., Iveranova, V.I., Kitaygorod-
skiy, A.I. and Pinsker, Z.G. 70-3-2-26/26

TITLE: The Fourth International Congress of Crystallography
(IV mezhunarodnyy kongress kristallografov) (Montreal,
July 10-19, 1957)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 2, pp 250 - 260
(USSR).

ABSTRACT: Outline of the scientific proceedings of the
conference.

Card 1/1

USCOMM-DO-60577

AUTHORS: Varfolomeyeva, L.A., Zhdanov, G.S. and Umanskiy, M.M. 70-3-3-23/36

TITLE: The Determination in Principal of the Structure of the Isomorphous Group of Compounds $[\text{C}(\text{NH}_2)_3][\text{M}(\text{H}_2\text{O})_6]_2, [\text{EO}_4]_2$

Where M = Al or Cr and E = S or Se (Printsipial'naya rasshifrovka struktury izomorfnoy gruppy soyedineniy $[\text{C}(\text{NH}_2)_3][\text{M}(\text{H}_2\text{O})_6]_2, [\text{EO}_4]_2$, M = Al, Cr; E = S, Se)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 368 - 371 (USSR).

ABSTRACT: From packing considerations possible positions for the various structural groups in compounds of the GASH type are suggested: $\text{M}(\text{H}_2\text{O})_6$ at (0,0,0), $(1/3, 2/3, z_1)$ and $(2/3, 1/3, z_1)$; $\text{C}(\text{NH}_2)_3$ at $(0,0,z_2)$, $(1/3, 2/3, 0)$ and $(2/3, 1/3, 0)$; EO_4 at $(1/3, 1/3, 1/4)$, $(0, 2/3, 1/4)$, $(2/3, 0, 1/4)$, $(2/3, 2/3, 3/4)$, $(0, 1/3, 3/4)$ and $(1/3, 0, 3/4)$. Patterson projections $P(x,y)$ and $P(x,z)$ were calculated from Weissenberg photographs for the compounds with (Al, S) and (Al, Se). These largely confirm the suggested model.

There are 3 figures and 3 tables and 3 References, 1 of which

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70-3-3-23/36
The Determination in Principal of the Structure of the Isomorphous
Group of Compounds $[C(NH_2)_3][M(H_2O)_6]_2$, $[EO_4]_2$ Where M = Al or Cr
and E = S or Se

is Soviet and 2 English.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet imeni
M.V. Lomonosova (Moscow State University imeni
M.V. Lomonosov)

SUBMITTED: February 22, 1958

Card 2/2

AUTHORS: Zhdanov, G.S., Zhuravlev, N.N., Kuz'min, R.N. and Soklakov, A.I. 70-3-3-26/36

TITLE: The Establishment by X-ray Crystallography of a New Compound Bi_3Rh in the System Bi-Rh (Rentgenograficheskoye ustanovleniye novogo soyedineniya Bi_3Rh v sisteme Bi-Rh)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 3, pp 373 - 374 (USSR).

ABSTRACT: Bi_4Rh has been supposed to occur in three polymorphic modifications α , β and γ . Goniometric and X-ray observations have been made on β - Bi_4Rh . Its habit is identical with that of Bi_3Ni and its cell dimensions $a=9.1$, $b=4.2$, $c=11.4$ Å are close to those of Bi_3Ni ($a=8.875$, $b=4.115$, $c=11.477$). Both have the space group $Pnma = D_{2h}^{16}$. $d_{obs.} = 10.7 \pm 0.2$ gm/cm³. gives Z nearly equal to 3 if the formula Bi_4Rh is used. It seems clear that the formula should be Bi_3Rh giving $Z=4$ and powder photographs also confirm this Card 1/2 resemblance to Bi_3Ni .

70-3-3-26/36

The Establishment by X-ray Crystallography of a New Compound Bi_3Rh
in the System Bi-Rh

There are 7 Soviet references.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet
imени M.V. Lomonosova (Moscow State University
imени M.V. Lomonosov)

SUBMITTED: July 11, 1957
Card 2/2

78-3-3-36/47

AUTHORS: Zhdanov, G. S. , Zhuravlev, N. N. , Kuz'min, R. N.

TITLE: An Investigation of the System Bi-Rh (Issledovaniye sistemy Bi-Rh)

PERIODICAL: Zhurnal Neorganicheskoy Khimii, 1958, Vol.3, Nr 3, pp.750-754 (USSR)

ABSTRACT: By X-ray analysis some compounds of bismuth and rhodium, especially Bi_4Rh and Bi_2Rh were investigated. The crystals of $\beta\text{-Bi}_4\text{Rh}$ and $\alpha\text{-Bi}_2\text{Rh}$ were investigated. The $\beta\text{-Bi}_4\text{Rh}$ -crystals are rhombic and have the following lattice constants: $a = 11,4 \pm 0,2 \text{ \AA}$, $b = 9,0 \pm 0,2 \text{ \AA}$, $c = 4,2 \pm 0,1 \text{ \AA}$. The density of the crystals is $\rho = 10,7 \pm 0,2 \text{ g/cm}^3$. The compound $\alpha\text{-Bi}_2\text{Rh}$ crystallizes in the monoclinic system with periods $a = 6,7 \text{ \AA}$, $b = 6,8 \text{ \AA}$, $c = 6,9 \text{ \AA}$. The system CoSb was investigated at the same time and on the basis of X-ray analyses it was found that $\alpha\text{-Bi}_2\text{Rh}$ and CoSb₂ are isomorphous compounds. The crystals $\alpha\text{-Bi}_2\text{Rh}$ can be classified with the structural type of markasite. During the melt-

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78-3-3-36/47

An Investigation of the System Bi-Rh

ing of antimony with cobalt, rhodium and iridium crystals of CoSb_2 , RhSb_2 and IrSb_2 were determined. These crystals have a monoclinic structure. The unit cells of the compounds CoSb_2 , RhSb_2 and IrSb_2 were calculated by the roentgengoniometric method.

CoSb_2 : $a = 6,5 \text{ \AA}$, $b = 6,5 \text{ \AA}$, $c = 6,5 \text{ \AA}$, $\beta = 118 \pm 1$, $\sigma = 8,3 \text{ g/cm}^3$, $Z = 4$

RhSb_2 : $a = 6,6 \text{ \AA}$, $b = 6,5 \text{ \AA}$, $c = 6,7 \text{ \AA}$, $\beta = 117 \pm 1$, $\sigma = 9,0 \text{ g/cm}^3$, $Z = 4$

IrSb_2 : $a = 6,6 \text{ \AA}$, $b = 6,5 \text{ \AA}$, $c = 6,7 \text{ \AA}$, $\beta = 116 \pm 1$, $\sigma = 10,85 \text{ g/cm}^3$, $Z = 4$

Bi_2Rh : $a = 6,7 \text{ \AA}$, $b = 6,8 \text{ \AA}$, $c = 6,9 \text{ \AA}$, $\beta = 117 \pm 2$, $\sigma = 12 \text{ g/cm}^3$, $Z = 4$

A new group of isomorphous compounds CoSb_2 , $\alpha\text{-RhSb}_2$, IrSb_2 , and $\alpha\text{-Bi}_2\text{Rh}$ was produced. There are 5 figures, 1 table, and 12 references, 11 of which are Soviet.

ASSOCIATION: Moskovskiy gosudarstvenny universitet im. M. V. Lomonosova
(Moscow State University imeni M. V. Lomonosov)

SUBMITTED: June 25, 1957

Card 2/2

ZHDANOV, G.S.

ZHURAVLEV, N.N.; ZHDANOV, G.S.

Study of the bismuth - palladium system. Zhur. neorg.khim. no.3:755
1958. (MIRA 11:4)

(Bibliography-Bismuth-palladium alloys)

SOV/70-3-4-11/26

AUTHORS: Venevtsev, Yu.N., Zhdanov, G.S., Solov'yev, S.P. and Zubov, Yu.A.

TITLE: The Internal Fields in Certain Ferro-electrics with Structures of the Perovskite Type (Vnutrenniye polya v nekotorykh segnetoelektrikakh so strukturoy tipa perovskita)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 4, pp 473-479 (USSR)

ABSTRACT: An analysis of the methods of calculating the internal field in ferro-electrics of the perovskite type is made. The internal fields and the spontaneous polarisation in the tetragonal modifications of BaTiO_3 and PbTiO_3 are calculated and the influence of certain cation parameters on these quantities is estimated. The structure was assumed, as a first approximation, to be built up of point charges and point dipoles. Kozlovskiy's method (Zh.Tekh. Fiz., Vol 21, Nr 11, p 1388, 1951) where the five different ions are attached to five separate sub-lattices was used. In BaTiO_3 the Ba ion was taken as the origin but in the PbTiO_3 the Ti in view of the reported displacements (Shirane, Pepinsky and Danner, Acta Crystall, 1956, Vol 9, p 131). Published polarisabilities were used.

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SOV/70-3-4-11/26

The Internal Fields in Certain Ferro-electrics with Structures of the Perovskite Type

As the effective ionic charges were not known, a coefficient of charging $\gamma (0 \leq \gamma \leq 1)$, identical for all ions, was introduced. If for BaTiO_3 , γ was taken as 1, then the calculated, spontaneous polarisation was twice the observed value. The value $\gamma = 1/2$ was therefore used for both BaTiO_3 and PbTiO_3 . The spontaneous polarisation when calculated was then near to the observed value and the internal fields were found to be BaTiO_3 : Ba, 0.04; Ti, 4.84; O_I , 3.66; O_{II} and O_{III} , 0.55. PbTiO_3 : Pb, 1.83; Ti, 8.62; O_I = 7.02; O_{II} and O_{III} , 2.23: in each case $\times 10^8$ V/cm. As the calculations were carried out with structure coefficients C_{ik} appropriate to a cubic structure, the approximation will be much better in the case of BaTiO_3 with $c/a=1.01$ than for PbTiO_3 with $c/a = 1.06$. The calculations were repeated with

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SOV/70-3-4-11/26

The Internal Fields in Certain Ferro-electrics with Structures of the Perovskite Type

variations in certain of the parameters. For BaTiO_3 , a was varied 4.2 and to 3.9 Å; α (polarisability) of the Ti was doubled and halved; the charge distribution was tried as $\text{Ba}^{+1/2}$, $\text{Ti}^{+2.5}$; the polarisability α_{Ba} of the Ba ions was doubled and halved. Similar variations were made for PbTiO_3 . The relative influences of the various contributory effects were then apparent. The effects on the spontaneous polarisation were also found. The results are compared with those of other authors. There are 3 tables and 33 references, 13 of which are Soviet, 15 English and 5 German.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova (Institute of Physical Chemistry imeni L. Ya. Karpov)

SUBMITTED: July 18, 1971.

Card 3/3

SOV/70-3-6-11/25

AUTHORS: Zhdanov, G.S., Zubov, V.G., Ivanov, A.T. and Firsova, M.M.

TITLE: On the Elastic Properties of Quartz Irradiated by Neutrons
(Ob uprugikh svoystvakh kvartsa, obluchennogo neytronami)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 6, pp 720-725 (USSR)

ABSTRACT: The elastic constants of quartz, irradiated in a reactor by fast neutrons, have been measured by the method of Bergmann and Schaeffer. After irradiation by $2 \cdot 10^{19}$ neutrons/cm² increasing errors which lay in the limits of 0.9 to 1.7% for a relative decrease in the density of quartz of 0.18% were found in the experiment for measuring the elastic constants. Comparison with the temperature variation of the elastic constants showed that the temperature and radiation changes in the elastic constants corresponding to the same change in density were sharply distinguished. The results agree qualitatively with the work of Mayer and Gigon (J. Phys. Rad., 1957, Vol 18, p 109) on the elastic moduli of irradiated quartz. Measurements were made on blocks about 20 x 20 x 4 mm cut perpendicular to the crystallographic axes. Four series each of three plates were used, careful controls being kept. The frequencies used were 8-10 Mc/s. Wittels and Sherill (Phil. Mag., 1957, Vol 48, p 24) contrasted the

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SOV/70-3-6-11/25

'On the Elastic Properties of Quartz Irradiated by Neutrons

changes in the elastic constants produced by thermal and radiation-produced expansion of the crystal lattice. Although qualitatively the anisotropy is the same the actual values for it are quite different. This is shown experimentally. The structural meaning of the results obtained is not discussed. Acknowledgments to Academician I.K. Kikoin and V.L. Karpov. There are 4 tables. There are 11 references, 3 of which are Soviet, 8 English.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet im.

M.V. Lomonosova (Moscow State University imeni

SUBMITTED: M.V. Lomonosov)
June 12, 1958

Card 2/2

SOV/70-3-6-19/25

AUTHOR: Venetsev, Yu.N. and Zhdanov, G.S.

TITLE: Crystal-chemical Analysis of the Temperature Phase
Transitions in Ferro- and Antiferro-electrics with
Structures of the Perovskite Type (Kristallokhimicheskiy
analiz temperaturnykh fazovykh perekhodov v segneto-i
antisegnetoelektrikakh so strukturoy tipa perovskita)

PERIODICAL: Kristallografiya, 1958, Vol 3, Nr 6, pp 751-752 (USSR)

ABSTRACT: It is known that the phase transitions undergone by
 BaTiO_3 and PbTiO_3 on cooling follow different sequences
(cubic-tetragonal-monoclinic-pseudorhombohedral and
cubic-rhombohedral-monoclinic, respectively). Perovskites
can be crystallo-chemically characterised by the values
of the tolerance factors t relating to their packings.
In BaTiO_3 t is greater than 1 and Ti^{4+} is the
ferro-electric ion. In PbZrO_3 t is less than 1 and the
 Pb^{2+} ion is the ferro-electric one. The co-ordinations and
situations of the two types of ion are quite different and
therefore so are the displacements which the structure can
undergo on cooling. Earlier observations on this point
by the present authors is recalled. In it the sequence

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Crystal-chemical Analysis of the Temperature Phase Transitions in
Ferro- and Antiferro-electrics with Structures of the Perovskite
Type

of deformations was discussed as a function of t
(Kristallografiya, 1957, Vol 2, p 233).

There 11 references, 7 of which are Soviet, 3 English
and 1 French.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(L.Ya. Karpov Physico-chemical Institute)

SUBMITTED: July 18, 1957

Card 2/2

SOV/78-3-11-19/23

AUTHORS: Epel'baum, V. A., Sevast'yanov, N. G., Gurevich, M. A.,
Ormont, B. F., Zhdanov, G. S.

TITLE: II. On the Phases Formed in the System Chromium-Boron (II. O
fazakh, obrazuyushchikhaya v sisteme khrom-bor)

PERIODICAL: Zhurnal neorganicheskoy khimii, 1958, Vol 3, Nr 11, pp 2545-2552
(USSR)

ABSTRACT: The compounds formed in the system chromium-boron are investigated. The investigations were carried out by means of chemical, radiographic, and metallographic methods in the region of the phase diagram of the system chromium-boron and in the range $\text{CrB}_{0,35}$ - CrB_3 . Purest boron (99,6%) produced by the thermal dissociation of diboranes served as initial components for the production of the chromium-boron phases. The results of the chemical and radiographic analyses of the samples were obtained by heating at 1150°C in vacuum and then at 1300°C in an argon atmosphere for 36 hours. The results are given in table 2. It was found that the γ -phase occurs with a rhombic lattice in the sample with a boron content of $\text{CrB}_{0,35}$ - $\text{CrB}_{0,58}$. In the samples

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SOV/78-3-11-19/23

II. On the Phases Formed in the System Chromium-Boron

with a boron content of $\text{CrB}_{0,41}-\text{CrB}_{0,51}$ only the γ -phase exists. In the samples with a boron content of $\text{CrB}_{0,55}-\text{CrB}_{1,05}$ the δ -phase (Cr_5B_3 -phase) is formed. In the samples with a boron content of $\text{CrB}_{0,59}-\text{CrB}_{0,63}$ only the δ -phase is formed. In the samples with a boron content of $\text{CrB}_{0,68}-\text{CrB}_{1,50}$ the ϵ -phase occurs (CrB with rhombic lattice). In the samples of the composition $\text{CrB}_{0,96}-\text{CrB}_{1,13}$ no other phases were found besides the ϵ -phase. In the sample with a boron content of $\text{CrB}_{1,20}-\text{CrB}_{1,90}$ a ζ -phase with rhombic lattice is formed. In the sample of the composition $\text{CrB}_{1,50}-\text{CrB}_{1,65}$ no other phases were found to exist besides the ζ -phase. In the samples with $\text{CrB}_{1,70}$ and $\text{CrB}_{1,90}$ only the η -phase is formed.

There are 2 figures, 5 tables, and 27 references, 1 of which is Soviet.

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24(2), 24(3)

AUTHORS:

Venevtsev, Yu. N., Zhdanov, G. S.,
Solov'yev, S. P.

SOV/48-22-12-17/33

TITLE:

Effect of Various Factors Upon the Curie Temperature of
Piezoelectrics With the Structure of the Perovskite Type
(Vliyaniye razlichnykh faktorov na temperaturu Kyuri
segnetoelektrikov so strukturoy tipa perovskita)

PERIODICAL:

Izvestiya Akademii nauk SSSR. Seriya fizicheskaya, 1958,
Vol 22, Nr 12, pp 1476-1482 (USSR)

ABSTRACT:

The question concerning the Curie (Kyuri) T_k temperature of piezoelectrics having a perovskite structure, was already investigated earlier (Refs 1-7 and 8-11). The analysis of these papers shows that there is no uniform opinion on this problem. The conclusions drawn from references 1-7 are based on the assumption that in the investigated piezo- and anti-piezoelectrics the cations of the B-type are piezoactive. Actually, in some piezoelectrics the B-cations and in others the A-cations are piezoactive (Refs 8, 9, 13). As it was already stated (Ref 10), the results given in references 1-7 must be subjected to further examinations, because of the reason mentioned above. The classifications, because of the piezo- and anti-piezoelectrics with perovskite structure depending on the

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Effect of Various Factors Upon the Curie Temperature
of Piezoelectrics With the Structure of the Perovskite Type

SOV/48-22-12-17/33

type of the piezoactive cation, as proposed in references 8, 9, 13 promotes the solution of the problem discussed. Therefore, they have been investigated again in this paper. It was attempted to explain the differences of the Curie temperature in piezoelectrics with perovskite structure in the same way, by using only such characteristics as polarizability, charges and radii. The degree of covalence of the bindings in the respective compounds was neglected. The authors started from an approximate theoretical estimation. They used the results from references 15, 16, determined in the investigation of the effect of various parameters of cations upon the internal field of piezoelectrics with perovskite structure. The conclusions drawn on the basis of theoretical estimations agree with the few experimental results obtained by the authors of this article and Sawaguchi (Ref 7). As soon as new experimental data will be obtained it will be possible to check also the theoretical results still improved.

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Effect of Various Factors Upon the Curie Temperature of Piezoelectrics with the Structure of the Perovskite Type SOV/48-22-12-17/33

There are 2 tables and 26 references, 12 of which are Soviet.

ASSOCIATION: Fiziko-khimicheskiy institut im. L. Ya. Karpova
(Physico-Chemical Institute imeni L. Ya. Karpov)

Card 3/3

VIASINKO, V.I.; ZHDANOV, G.S.

Using calculating machines for radiographic studies. Zav. lab. 24
no.5:634-636 '58. (MIRA 11:6)

1. Fiziko-khimicheskiy institut im. L.Ya. Karpova.
(Radiography) (Electronic calculating machines)

AUTHORS: Zhdanov, G. S., Kefeli, L. M. 76-32-3-26/43

TITLE: An Investigation of the Texture of Copper Obtained in the Leaching of CuAl_2 by the Method of Pole Figures
(Issledovaniye tekstury medi pri vyzhchelachivaniyu CuAl_2 metodom polyusnykh figur)

PERIODICAL: Zhurnal Fizicheskoy Khimii, 1958, Vol 32, Nr 3, pp 666 - 669 (USSR)

ABSTRACT: It was noticed that copper in a polycrystalline, dispersed form remains behind in the leaching out of aluminium from alloys. Radiographic investigations showed condensed spots which indicate a certain orientation of the copper crystals. The method mentioned in the title was employed for the investigation of the crystal orientation, because it is convenient and objective. A schematically drawn representation of the arrangement in the method of investigation according to the pole figures is given. From the data of the method of investigation, follows that the crystal sample was leached for 1-10 minutes with a 20% lye at 40-50°C. For obtaining

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76-32-3-26/43

An Investigation of the Texture of Copper Obtained in the Leaching of CuAl₂ by the method of Pole Figures

the polar points, a series of X-ray photographs was taken, where the sample was turned in a circle by 10° (around the 001 axis). From the considerations, it follows that in leaching out the monocrystal CuAl₂, on the one hand, the formation of polycrystalline CuAl₂ takes place, and on the other hand that of copper, where the two crystals form a texture. The texture of copper is characterized by the following data: CuAl₂ /001/, /100/, /010/; Cu /011/, ~ /111/, ~ /111/. There are 9 figures, 3 tables, and 6 references, 3 of which are Soviet.

SUBMITTED: December 11, 1956

Card 2/2

56-34-4-5/6o

AUTHORS: Zhuravlev, N. N., Mingazin, T. A., Zhdanov, G. S.

TITLE: The Structure of Superconductors. XII (Struktura sverkhprovodnikov. XII) The Investigation of Bismuth - Rubidium Alloys (Issledovaniye splavov vismuta s rubidiem)

PERIODICAL: Zhurnal eksperimental'noy i teoreticheskoy fiziki, 1958, Vol. 34, Nr 4, pp. 820 - 826 (USSR)

ABSTRACT: According to thermal, microscopical, and radiographic data the test diagram (probnaya diagramma) of the fusibility of the system Bi-Rb is constructed. The investigation of this system is connected with the solution of various methodical problems. The main difficulties mainly are connected with the high chemical activity of metallic rubidium and also with the great difference of the physical-chemical properties of bismuth and rubidium. The whole investigation was performed at small quantities ($\sim 3g$) of rubidium which required the working out of micromethods for the production of the alloys and their physical-chemical analysis. First the production

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The Structure of Superconductors. XII. The Investigation of Bismuth-Rubidium Alloys

56-34-4-5/60

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of the alloys is discussed, the apparatus used for this are discussed by means of figures. The melting was performed in small resistance furnaces. Then the authors report on the thermal analysis of the alloys. The curves of heating and cooling were taken by an automatic electron potentiometer unto a temperature of 50 - 100°C. The results of the thermal analysis obtained are illustrated in a diagram and subsequently discussed. At the bismuth-rich alloys (to the composition Bi_2Rb) also a metallographical investigation was performed. According to this the number of the crystals of the compound Bi_2Rb increases with increasing rubidium content in the alloy. The alloy with 15,8 per cent by weight rubidium according to its composition resembles the compound Bi_2Rb (17 per cent by weight;) it contains a small quantity of eutectic and is almost homogeneous. In the system Bi-Rb the various phases differ by their color. Then the authors report on the determination of the structure of the superconductive compound Bi_2Rb . By

The Structure of Superconductors. XII. The Investigation of Bismuth-Rubidium Alloys

56-34-4-5/60

exact determination of the lattice period of Bi_2Rb the value $a = 9,590 \pm 0,002 \text{ kX}$ was obtained. The distances between the lattice planes, computed from these data agree well with the measured results. The Rb atoms in the structure of the Bi_2Rb are distributed according to the diamond law. Some conclusions are: In the system bismuth-rubidium 4 compounds were stated: Bi_2Rb , BiRb_3 , and two compounds of the probable composition Bi_2Rb_3 and BiRb_2 . The maxima in the fusibility diagram correspond to the compounds Bi_2Rb and BiRb_3 . These compounds form in the fusion of the components with high heat emission. The two other compounds form according to the peritectic reaction. The superconductive compound Bi_2Rb crystallizes in isometric syngony with $a = 9,590 \pm 0,002 \text{ kX}$ and has a structure of the type of Cu_2Mg . The increase of the minimum interatomic distances in the Bi_2Rb leads to an increase of the temperature of the transition into the superconductive state. Finally the author

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The Structure of Superconductors. XII. The Investigation of Bismuth-Rubidium Alloys

56-34-4-5/60

thanks Professor N. Ye. Alekseyevskiy for his valuable advice in the performance of this work, and R. N. Kuz'min for his assistance in the performance of the experiments. There are 6 figures and 10 references, 9 of which are Soviet.

ASSOCIATION: Moskovskiy gosudarstvennyy universitet (Moscow State University)

SUBMITTED: November 15, 1957

1. Bismuth alloys--Analysis 2. Superconductors--Structural analysis

Card 4/4

AUTHORS: Gol'der, G. A., Zhdanov, G. S.

20-118-6-23/43

TITLE: A Radiographic Structural Examination of Naphthazarine
(Rentgenostrukturnoye issledovaniye naftazarina)

PERIODICAL: Doklady Akademii Nauk SSSR, 1958, Vol. 118, Nr 6,
pp. 1131-1133 (USSR).

ABSTRACT: Naphthazarine is widely spread amongst the hydroxy ketone dyes,
the naphthoquinone-derivates (5,8-dioxy-1,4 naphthaquinone).
The authors give a survey on the literature of the radiographic
investigation (reference 1), as well as of the investigation of
magnetic anisotropy (reference 2). There exist 2 modifications of
naphthazarine: 1) dark-green pins, 2) dark-red prisms; the
authors obtained a third modification by crystallization in ben-
zene, viz. 3) light-red platelets. Their radiographic data are
given in table 1. If and when all 3 modifications precipitate from
the solution, well-faceted crystals of the 3rd modification occur
most frequently. The modifications 1) and 2) were formed by
sublimation. The belonging of the crystals of the 1st modification
to the spatial group $C_{2h}^1 = P2_1/c$ and the presence of 2 molecules
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A Radiographic Structural Examination of
Naphthazarine

20-118-6-23/43

in the elementary mesh conform the assumption (reference 1) that a center of symmetry exists in the molecule of the crystals of the 1st modification. The introduction of an inner hydrogen compound O . . . H-O in the conjugated bond-system must have caused an essential change of the π -electronic interaction in the whole molecule. This must, in return, lead to a redistribution of the electronic density in the molecule. A complete radiographic analysis of the crystals of this modification was interesting therefore. The lengths of the bonds between the atoms in the molecule were computed (II) from the atomic coordinates computed from ρ (OKL)(table 2). The computations of the distances between the atoms were carried out under the assumption that the molecule of the surface yz lies parallel. The angle formed by the bond-line $C_9 - C_{10}$ with the y-axis of the mesh, is 50° . The smallest distance between the carbon- and oxygen-atoms in various molecules is 3,10 Å. The results of the radiographic structural analysis confirm the presence of a center of symmetry in the 1st modification of naphthazarine. As mentioned above, all 3 modifications precipitate simultaneously with the crystallization of the solution: 2 centro-symmetrical ones (A), and a none-centro-symmetrical one (B). The

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A Radiographic Structural Examination of Naphthazarine 20-118-6-23/43

recrystallization of each of these modifications leads in return to the formation of all these 3 modifications, though one of them prevails largely. It may thus be presumed that the transition of an isomer of an A-structure into an isomer of a B-structure (and viceversa) takes place. This transition is explained with scheme III and was presumed in reference 4. The orientation in space of the molecule in the yz-surface achieved by the authors, is very similar to that for the centro-symmetrical modification 2) given in reference 3. A three-dimensional synthesis is required for determining the 3rd coordinate x and for defining precisely the obtained results. There are 1 figure, 2 tables, and 4 references, 1 of which is Slavic.

ASSOCIATION: Physico-Chemical Institute imeni L. Ya. Karpov
(Fiziko-khimicheskiy institut im. L. Ya. Karpova)
PRESENTED: November 20, 1957, by N. V. Belov, Academician.
SUBMITTED: August 16, 1957.
Card 3/4

"APPROVED FOR RELEASE: 07/19/2001

CIA-RDP86-00513R002064620006-5

A Radiographic Structural Examination of
Naphthazarine

20-118-6-23/43

Card 4/4

APPROVED FOR RELEASE: 07/19/2001

CIA-RDP86-00513R002064620006-5"

20-119-1-23/52

AUTHORS: Dokunikhin, N. S., Gol'der, G. A., Zhdanov, G. S.

TITLE: The Radiographic Investigation of 1,4-di-Anilido-Anthraquinone and 1,4-Dimesido-Anthraquinone (Rentgenograficheskoye issledovaniye 1,4-dianilidoantrakhinona i 1,4-dimezidoantrakhinona)

PERIODICAL: Doklady Akademii Nauk SSSR, 1958, Vol. 119, Nr 1,
pp. 87 - 89 (USSR)

ABSTRACT: Sulfo acids of 1,4-di-(arylamino)-anthraquinone form an important group of solid dyes for wool. The majority of the 1,4-di-(arylamino)-substitutes of anthraquinone are green. An exception is made by the derivatives in which all hydrogen atoms, in an ortho-position, of the aryl-residues are substituted. Such compounds as well as the corresponding alkyl-amino-and hydro-aryl-amino-derivatives have an intensive bright-blue color. In the presence of methyl-ethyl-groups or of bromine atoms in all ortho-positions of the phenyl residues or in the position of 2,3-anthraquinone respectively

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20-119-1-23/52

The Radiographic Investigation of 1,4-di-Anilido-Anthraquinone and
1,4-Dimesido-Anthraquinone

the absorption in the short-wave range of light is absent and the chief maximum is displaced in the direction of the short waves, when the light absorption is measured by CCl_4 -solutions of 1,4-di-(arylamino)-anthraquinone in the visible and in the ultraviolet range of the spectrum (Reference 1). The appearance of an additional principal band and the deepening of the principal band in the absence of spatial disturbances might logically be considered a consequence of the coplanarity of the molecule. This is also indicated by the comparison of the absorption frequencies in the infrared spectral region (Reference 2). These data indicate the weakening of the inner-molecular hydrogen bond of the carbonyl-oxygen with the hydrogen of the amino groups in the presence of spatial obstacles of a coplanar orientation of the benzene nuclei. This bond is weakened by the increased distance due to the leaving of the plane of the anthraquinone-

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20-119-1-23/52

The Radiographic Investigation of 1,4-di-Anilido-Anthraquinone and
1,4-Dimesido-Anthraquinone

cycles by hydrogen and is caused by the disturbance of the conjugation -system (Reference 3). It would be desirable to find a direct proof of the flat structure of the molecules of 1,4-di-(aryl amino)-anthraquinone in the absence of spatial difficulties. For the purpose of deciding the problem of coplanarity of the benzene nuclei with the plane of the basic part of the molecule, crystals of both compounds mentioned in the title were radiographically measured. The results are given in table 1. From the dimensions of the elementary cell of the first compound can be assumed that the basic part of the molecule is here entirely or almost parallel with the ac-plane, as axis b is the shortest one (8,73 Å). From the conditions of symmetry of the spatial group

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$$C_{2h}^5 = P2_1/c$$

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The Radiographic Investigation of 1,4-di-Anilido-Anthraquinone and
1,4-Dimesido-Anthraquinone

follows that a slip plane with a displacement along axis c runs vertical to axis b. Thereby the 4 molecules occurring in the unit cell are orientated in layers which are perpendicular to axis b. A variant of this orientation is shown by figure 1. It admits a slight turn of the benzene nucleus in relation to the other part of the molecule as well as a certain possible turn of the entire molecule in relation to the plane ac. Thus the packing of the molecules in the crystal does not require an additional change of the angle of rotation of the benzene nucleus as compared to the free molecule. The shortest axis in the crystal of the second compound is the a-axis (7,98 Å). Its length corresponds to the dimensions of the benzene nucleus and to the CH_3 -groups connected with it (8,8 Å). A solid packing of molecules in the crystal and the fulfilment of the conditions of symmetry of the spatial group for molecules of the second compound

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20-119-1-23/52

The Radiographic Investigation of 1,4-di-Anilido-Anthraquinone and
1,4-Dimesido-Anthraquinone

of the methyl groups to all meta-positions of the benzene nucleus creates so great spatial difficulties that the coming out with the anthraquinone cycles from the coplanarity amounts to almost 90°. Thereby the inner-molecular linkage is considerably weakened. There are 2 figures, 1 table, and 5 references, all of which are Soviet.

ASSOCIATION: Nauchno-issledovatel'skiy institut organicheskikh poluproduktov i krasiteley im. K. Ye. Voroshilova (Scientific Research Institute of Organic Semiproducts and Dyes imeni K. Ye. Voroshilova). Nauchno-issledovatel'skiy fiziko-khimicheskiy institut im. L. Ya. Karpova (Scientific Physical-Chemical Research Institute imeni L. Ya. Karpova)

PRESENTED: November 20, 1957, by N. V. Belov, Member, Academy of Sciences, USSR

SUBMITTED: August 16, 1957

Card 6/6

ZHDANOV, G.S.

БИБИКОВ, С. А. И. СОЛОДЧИЙ, Sergey Pavlovich; ВИНОГДРЯН, Тарас Николаевич;
СИДОРЧУК, В. В.

"Internal Fields in the Orthorhombic Modification of Barium Titanate"

A report presented at Symposium of the International Union of Crystallography Leningrad, 21-27 May 1977

APPROVED FOR RELEASE: 07/19/2001 CIA-RDP86-00513R002064620006-5"

VLASENKO, V.I., kand.tekhn.nauk; ZHDANOV, G.S., prof.; DEMENT'YEV,
A.M., inzh.; ANTONOVA, I.M., inzh.

Use of a ferrite matrix in a method for forming numbers.
[Trudy] MVTU no.2:64-69 '59. (MIRA 13:5)
(Electronic calculating machines)

24,7700
24 (3), 10 (6)

68047

SOV/55-59-3-15/32

AUTHORS: Alekseyevskiy, N. Ye., Zhdanov, G. S., Zhuravlev, N. N.TITLE: The Problem of the Superconductivity of Compounds of Bismuth With Alkali MetalsPERIODICAL: Vestnik Moskovskogo universiteta. Seriya matematiki, mekhaniki, astronomii, fiziki, khimii, 1959, Nr 3, pp 113 - 115 (USSR)

ABSTRACT: By analysis of the critical temperature of bismuth-alkali compounds a linear dependence between the critical temperature T_c of the compound and the atomic radius of the alkali metal was found. This linear dependence does not hold for the LiBi compound; it possibly holds for the compounds with alkaline earth metals. A comparison between T_c and the atomic radius is quite permitted for the isomorphic compounds KBi_2 , $RbBi_2$, $CsBi_2$, but less for $NaBi$, which has a different type of lattice. With an increase in the critical temperature T_c the minimum interatomic spacings in the transition from KBi_2 to $CsBi_2$ increase, the dependence between the minimum distance and T_c being linear. By means of a relationship between dH_k/dT and γ (the coefficients

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5-(4), 24-(3)

68048

SOV/55-59-3-16/32

AUTHORS:

Zhuravlev, N. N., Zhdanov, G. S., Alekseyevskiy, N. Ye;

TITLE:

The Crystal Chemistry of Superconductive Bismuth Compounds

PERIODICAL:

Vestnik Moskovskogo universiteta. Seriya matematiki, mekhaniki, astronomii, fiziki, khimii, 1959, Nr 3, pp 117 - 127 (USSR)

ABSTRACT:

The present paper deals with some results obtained by an analysis of the crystallo-chemical data found by the authors concerning the structure of superconductive bismuth compounds. A comparison between the superconductive properties with crystallo-chemical data was carried out on the basis of known results determined in most cases by N. Ye. Alekseyevskiy (Refs. 20 - 35) at the Institut fizicheskikh problem AN SSSR (Institute for Physical Problems of the AS USSR). The first part of the present paper deals with 1) the capability of bismuth to form compounds with various elements of the periodic system and 2) with the electric properties of these compounds. Among other things the existence of the compounds K_9Bi_7 , K_3Bi_2 , Rb_3Bi_2 , Rb_2Bi , and Cs_2Bi is supposed. It may be that the compounds $CeBi_2IrBi$ and β - $LiBi$ are superconductive. With the

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The Crystal Chemistry of Superconductive Bismuth Compounds SOV/55-59-3-16/32

of T_c . Bismuth compounds with transition metals show the reverse effect. The minimum interatomic spacings bismuth-bismuth vary within a wide range in the case of the various bismuth compounds. Bismuth compounds with small and also with large bismuth-bismuth spacings are not superconductive, but all compounds in which bismuth-bismuth spacings are within the "optimum" interval (3.1 to 3.8 Å) are superconductive. The superconductive modification of bismuth probably has a face-centered elementary cell. A large table shows the atomic-crystalline structural properties of bismuth compounds with non-superconductive elements. The experiments made by N. B. Brandt (Ref 56) are indicative of a decrease of the anisotropy of the crystal structure of ordinary bismuth in the case of compression. There are 3 figures, 4 tables, and 56 references, 40 of which are Soviet.

ASSOCIATION: Kafedra fiziki tverdogo tela (Chair for Solid-state Physics)

SUBMITTED: February 27, 1959

Card 3/3

4

AUTHORS: Yezhkova, Z.I., Zhdanov, G.S. and Umanskiy, M.M. SOV/70-4-2-24/36

TITLE: The Thermal Expansion of Crystals of Triglycinesulphate
in the Region of Their Ferro-electric Transition
(Termicheskoye rasshireniye kristalla triglycinesul'fata
v oblasti segnetoelektricheskogo perekhoda)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 249-253 (USSR)

ABSTRACT: $(\text{CH}_2\text{NH}_2\text{COOH})_3\text{H}_2\text{SO}_4$ is monoclinic with $a = 9.15$,
 $b = 12.69$, $c = 5.73 \pm 0.03 \text{ \AA}$, $\beta = 105^{\circ}40' \pm 20'$ with
space group $P2_1$ below the Curie point at 47° and
 $P2_1/m$ above. $Z = 2$ $d_{\text{obs}} = 1.69$ and the ferro-electric
axis is $[010]$ (according to Wood and Holden - Ref 6).
Here, the thermal expansion of single crystals has been
measured from X-ray single-crystal oscillation photographs.
The most accurate values were obtained from $d_{900}(\text{FeK}_\alpha)$
with $\Theta \sim 81^{\circ}$, $d_{007}(\text{Cu K}_\alpha)$ with $\Theta \sim 78^{\circ}$,
 $d_{505}(\text{Ni K}_\alpha)$ with $\Theta \sim 81^{\circ}$ and $d_{0,14,0}(\text{Co K}_\alpha)$ with
 $\Theta \sim 83^{\circ}$. Absorption corrections (for the 0.4 mm dia

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SOV70-4-2-24/36

The Thermal Expansion of Crystals of Triglycinesulphate in the Region
of Their Ferro-electric Transition

crystal were not applied. The accuracy was estimated at ± 0.0015 kX. β was calculated. The components of the thermal expansion tensor (principal components) were calculated as follows, where φ is the angle of α_{11} to the a axis of the crystal. At 25°C $\alpha_{11} = -37$, $\alpha_{22} = 5$, $\alpha_{33} = 142$ (in each case $\text{deg}^{-1} \times 10^{-6}$) and $\varphi = 22^\circ$. At 42.5°C $\alpha_{11} = -20$, $\alpha_{22} = 36.5$, $\alpha_{33} = 119$ and $\varphi = 7^\circ 20'$. Between 51 and 75°C $\alpha_{11} = 40$, $\alpha_{22} = 64$, $\alpha_{33} = -12.5$ and $\varphi = 5^\circ 40'$. The cell volume changes smoothly over the whole temperature range. It is concluded that the phase transition is of the second order and that a marked redistribution of the hydrogen bonds parallel to the ac plane occurs at the ferro-electric transition. There are 4 figures, 3 tables and 7 references, 2 of which are Soviet, 4 English and 1 international.

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SOV/70-4-2-24/36
The Thermal Expansion of Crystals of Triglycinesulphate in the
Region of Their Ferro-electric Transition

ASSOCIATION: Moskovskiy gosudarstvennyy universitet imeni
M.V. Lomonosova (Moscow State University imeni
M.V. Lomonosov)

SUBMITTED: October 13, 1958

Card 3/3

AUTHORS: Venevtsev, Yu.N., Zhdanov, G.S., Sov^{70-4-2-26/36}, Solov'yev, S.P. and Ivanova, V.V.

TITLE: On Internal Fields in Ferroelectric $PbTiO_3$ (O vnutrennikh polyakh v segnetoelektrike $PbTiO_3$)

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 2, pp 255-257 (USSR)

ABSTRACT: Calculations of the internal fields in $PbTiO_3$ crystals

have been made by the Madelung-Hagedorn method (R. Hagedorn - Ref 3) which is more accurate than Kozlovskiy's method used before, according to the work of Yu.N. Venevtsev et al (Ref 1). These fields E_i are

Pb 1.4, Ti 6.9, O_I 6.1 and O_{II} , O_{III} 1.8×10^8 V/cm.

The contributions of the separate ions to the spontaneous polarisation of 81×10^{-6} coulomb/cm² are tabulated. The internal fields for model crystals of the $PbTiO_3$ type but with ions of different polarisability are similarly calculated. For $BaTiO_3$ the calculations by both methods

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On Internal Fields in Ferroelectric $PbTiO_3$

are in good quantitative agreement. Graphical examination of the parameters affecting the internal fields show their relative importance. In order they are: 1) lattice period; 2) charge on the ferroelectric cation; 3) polarisability of the ions of the oxygen octahedra; 4) polarisability of the ferroelectric cation; 5) polarisability of the non-ferroelectric cation. There are 1 figure, 2 tables and 5 references, 4 of which are Soviet and 1 German.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(Physical-Chemical Institute im. L. Ya. Karpov)

SUBMITTED: November 14, 1958

Card 2/2

AUTHORS: Venevtsev, Yu.N., Solov'yev, S.P. and Zhdanov, G.S. SOV/70-4-4-17/34

TITLE: On the Structural Coefficients of the Internal Field in Ferroelectrics of the Perovskite Type

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 4, pp 575-578 (USSR)

ABSTRACT: The notation is carried over from an article by the same authors (Ref 1). The values of the projection of the structural coefficients $S_1(x, y, z) = C_{ik}$ for different orientations (cube edges, face or body diagonals) of the dipoles in a cubic perovskite-type cell are tabulated in terms of P and Q . ($P = -15.04102$ and $Q = 4.33387$). The coefficients C_{ik} are dimensionless and numerically equal to the field strength, additional to the Lorentz field, due to the sub-lattice of unit dipoles of the k -th sort of ion and acting on the i -th sort of ion. The derivation of expressions such as :

$$S_2(0, 1/2, 1/2) = S_3(0, 1/2, 1/2) = a/\sqrt{3}$$

Card1/2 and

On the Structural Coefficients of the Internal Field in Ferro-
electrics of the Perovskite Type

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$S_2(1/2, 0, 0) = S_3(1/2, 0, 0) = P/\sqrt{3}$
is given but all the other values are tabulated.
There are 1 table and 1 Soviet reference.

ASSOCIATION: Fiziko-khimicheskiy institut im. L.Ya. Karpova
(Physico-chemical Institute imeni L. Ya. Karpov)

SUBMITTED: June 23, 1958

Card 2/2

24.7000

75994
SOV/70-4-5-16/36

AUTHORS: Yezhkova, Z. I., Zhdanov, G. S., Umanskiy, M. M.

TITLE: An X-Ray Diffraction Method for the Determination of the Thermal Expansion Tensors of the Crystals of Low Symmetry

PERIODICAL: Kristallografiya, 1959, Vol 4, Nr 5, pp 723-726
(USSR)

ABSTRACT: If the principal expansion directions, that determine the diagonal tensor α_{11} , are the orthogonal coordinate axes X' , Y' , Z' , the thermal-expansion coefficient in 1 direction is described by

$$\Delta_1 = \alpha_{11}c_{11}^2 + \alpha_{22}c_{21}^2 + \alpha_{33}c_{31}^2 \quad (3)$$

where c_{11} , c_{21} , c_{31} are direction cosines of 1. In cubic, tetragonal, hexagonal, rhombohedral and orthorhombic crystals, the expansion coefficients along one, two, or three crystallographic axes suffice to determine the tensor. In monoclinic crystals only

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An X-Ray Diffraction Method for the Determination of the Thermal Expansion Tensors of the Crystals of Low Symmetry

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$\langle 010 \rangle$ coincides with one of the expansion tensor components, and in triclinic crystals, none. Consequently, the determination of the thermal expansion tensor in monoclinic crystals requires the data on the expansion of interplanar spacings of 4 different hkl , more conveniently of d_{010} and of three spacings of d_{hkl} type, and in triclinic crystals of 6 different spacings, more conveniently of d_{100} , d_{010} , d_{001} , d_{110} , d_{101} , d_{011} . In a coordinate system X,Y,Z of which the first two are parallel to $\langle 100 \rangle$ and $\langle 010 \rangle$, respectively, and the third is normal to (010) , the thermal expansion of a monoclinic crystal in the direction parallel to (010) and under angle φ to the X axis is described by

$$\Delta_\varphi = a_{11} \cos^2 \varphi + a_{33} \sin^2 \varphi + 2a_{13} \cos \varphi \cdot \sin \varphi. \quad (2a)$$

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Here, the values are determined by the following three

An X-Ray Diffraction Method for the Determination of the Thermal Expansion Tensors of the Crystals of Low Symmetry

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equations:

$$2\alpha_{11} = a_{11} + a_{33} + \frac{a_{11} - a_{33}}{\cos 2\psi}; \quad 2\alpha_{33} = a_{11} + a_{33} - \frac{a_{11} - a_{33}}{\cos 2\psi}$$

$$\tan 2\varphi = 2\alpha_{13} : (a_{11} - a_{33})$$

where ψ is the angle between α_{11} and X-axis. The orthogonal coordinate axes X, Y, Z for triclinic crystals must be chosen as follows: X coincides with the reciprocal-lattice axis a^* , Y is in the a^*b^* plane, and Z is normal to that plane and coincides with c-axis. Referred to this set of coordinates, the thermal-expansion tensor is described by the expression:

$$\alpha_{ik} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \quad (1)$$

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An X-Ray Diffraction Method for the Determination of the Thermal Expansion Tensors of the Crystals of Low Symmetry

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the 6 subscripts in which are determined by the thermal expansions of the mentioned 6 interplanar spacings as follows:

$$\begin{aligned}
 \Delta_{100} &= a_{11}, \\
 \Delta_{010} &= a_{11} \cos^2 \gamma + a_{22} \sin^2 \gamma + 2a_{12} \cos \gamma \sin \gamma, \\
 \Delta_{110} &= a_{11} \cos^2 (a' H_{110}) + a_{22} \sin^2 (a' H_{110}) + 2a_{12} \sin (a' H_{110}) \cos (a' H_{110}), \\
 \Delta_{001} &= a_{11} \cos^2 \beta + a_{22} \cos^2 (c' Y) + a_{33} \cos^2 (c' H_{001}) + 2a_{12} \cos \beta \cos (b' Y) + \\
 &\quad + 2a_{13} \cos \beta \cos (c' c) + 2a_{23} \cos (c' Y) \cos (c' c), \\
 \Delta_{101} &= a_{11} \cos^2 (a' H_{101}) + a_{22} \cos^2 (H_{101} Y) + a_{33} \cos^2 (H_{101} c) + \\
 &\quad + 2a_{12} \cos (a' H_{101}) \cos (H_{101} Y) + 2a_{13} \cos (H_{101} a') \cos (H_{101} c) + \\
 &\quad + 2a_{23} \cos (H_{101} Y) \cos (H_{101} c), \\
 \Delta_{011} &= a_{11} \cos^2 (H_{011} a') + a_{22} \cos^2 (H_{011} Y) + a_{33} \cos^2 (H_{011} c) + \\
 &\quad + 2a_{12} \cos (H_{011} a') \cos (H_{011} Y) + 2a_{13} \cos (H_{011} a') \cos (H_{011} c) + \\
 &\quad + 2a_{23} \cos (H_{011} Y) \cos (H_{011} c).
 \end{aligned} \tag{5}$$

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An X-Ray Diffraction Method for the Determination of the Thermal Expansion Tensors of the Crystals of Low Symmetry

75994

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h_{hkl} means reciprocal-lattice vector; $\alpha^*, \beta^*, \gamma^*$ and other angles can be expressed in terms of the crystallographic interaxial angles according to known equations. The transformation of the found tensor a_{ik} into the diagonal tensor a'_{ik} , i.e. reference of the tensor to the set of X', Y', Z' axes, is achieved using

$$D(\alpha) = -\alpha^3 + S_1\alpha^2 - S_2\alpha + S_3. \quad (6)$$

$$S_1 = a_{11} + a_{22} + a_{33},$$

$$S_2 = \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{13} \\ a_{13} & a_{33} \end{vmatrix} + \begin{vmatrix} a_{22} & a_{23} \\ a_{23} & a_{33} \end{vmatrix},$$

$$S_3 = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{vmatrix}.$$

There are 3 figures; and 5 references, 4 Soviet, 1 U.K.
The U.K. reference is: Y. A. Wooster, Textbook on
Crystalphysics, Oxford, 1938.

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An X-Ray Diffraction Method for the Determination of the Thermal Expansion Tensors of the Crystals of Low Symmetry 75994
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AUTHORS: Zhdanov, G. S., Solov'yev, S. P., Venevtsev, Yu. N.,
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TITLE: Internal Fields in the Orthorhombic Modification of
BaTiO₃

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ABSTRACT: Internal fields in orthorhombic (pseudomonoclinic) barium titanate are computed according to ionic-displacement data reported in Phys. Rev., 105, 3, 856, 1957. Computations are based on the assumption that point ionic charges are displaced parallel to the edges of monoclinic unit cells, twice as small as orthorhombic cells, and are superposed by the similarly displaced point dipole moments. The latter's magnitude is determined as the product of ionic polarization and the affecting internal field. The known equation:

$$E_x = p_x \sum \frac{2x_i^2 - y_i^2 - z_i^2}{(x_i^2 + y_i^2 + z_i^2)^{3/2}} + p_y \sum \frac{3x_i y_i}{(x_i^2 + y_i^2 + z_i^2)^{3/2}} + p_z \sum \frac{3x_i z_i}{(x_i^2 + y_i^2 + z_i^2)^{3/2}}$$

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